

# The Role of Electron-Hole Symmetry Breaking in the Kondo Problems <sup>\*</sup>

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*In studying the different Kondo problems it is generally assumed that breaking the electron-hole symmetry does not affect the perturbative infrared divergencies. It is shown here that, in contrast, breaking that symmetry may in some cases lead to observable modifications while in other cases it does not.*

*PACS numbers: 72.10Fk, 72.15Qm, 75.20Hr, 71.27+a*

## 1. INTRODUCTION

The heart of the Kondo phenomena is in the infrared divergences or the orthogonality catastrophe. Those phenomena occur in the neighborhood of the Fermi energy. Thus, breaking the electron-hole symmetry on the large energy scale of the conduction band width does not enter directly. In the first iterations of the scaling at large energy scale that may, however, induce non-universal effects.

In the first part of this paper, the spin Kondo problem with asymmetric bandwidth cutoff is studied. The results are somewhat unexpected, as the generated potential scattering in the intermediate energy region plays a relevant role in the scaling equations, which is not the case for symmetric bands.

Two examples are presented where the breaking of the electron-hole symmetry leads to instabilities of the scaling trajectories. The first example

<sup>\*</sup>Dedicated to Peter Wolfle on the occasion of his 60th birthday who is an old-time friend of us and whose work has been always stimulating for us.

is a two-level impurity model with commutative couplings where there is an additional potential scattering at the impurity site which generates non-commutative terms in the Hamiltonian. The other one is a two-level system with two-channel Kondo behavior, where the spin degeneracy is broken by spin-orbit scatterings in the neighborhood of the impurity atom. In both cases the energy splitting or direct tunneling generates the non-universal terms via the asymmetric band, but as those parameters also play the role of the infrared cutoff in the scaling the new fixed point cannot be reached.

In the last part, the tunneling impurity model with higher excitations in the potential well is discussed. The question of physical realization is not raised, it is only shown that the behavior in the high energy region of the scaling can be modified by the electron-hole symmetry breaking. This may change the parameters entering into the low energy physics.

## 2. ELECTRON-HOLE SYMMETRY

Treating the Kondo problem in the framework of the logarithmic approximation, the following formulas are used for the energy integrals

$$\int \rho(\varepsilon) \frac{n_F(\varepsilon)}{\omega - \varepsilon} d\varepsilon \rightarrow \rho_0 \log \frac{\text{Max}(kT, |\omega|)}{D} , \quad (1)$$

and for  $|\omega| \ll D$

$$\int \rho(\varepsilon) \frac{1}{\omega - \varepsilon} d\varepsilon \rightarrow \rho_0 \int_{-D}^D \frac{1}{\omega - \varepsilon} d\varepsilon \approx O\left(\frac{|\omega|}{D}\right) \rightarrow 0 , \quad (2)$$

where  $\omega$  is the energy variable,  $n_F$  is the Fermi distribution function, and  $\rho(\varepsilon)$  is the conduction electron density of states which is approximated by a constant  $\rho_0$  inside the region  $-D < \varepsilon < D$ ,  $D$  being an energy cutoff, e.g. the bandwidth. Those approximations do not affect the infrared divergent parts proportional to  $\log(\omega)$ , but the non-diverging terms can strongly depend on any deviation from those. Furthermore, the dependence on the wave number  $k(\varepsilon)$  for an electron with energy  $\varepsilon$  is replaced by the value at the Fermi energy  $k_F$ , thus

$$k(\varepsilon) = k_F + \varepsilon v_F \rightarrow k_F , \quad (3)$$

where  $v_F$  is the Fermi velocity. All of these approximations can be considered to be due to the electron-hole symmetry (e-h.s.).

That symmetry can be broken e.g. by introducing an energy dependent density of states (see e.g. Ref.1)

$$\rho(\varepsilon) = \rho_0 \left(1 + \alpha \frac{\varepsilon}{D}\right) , \quad (4)$$

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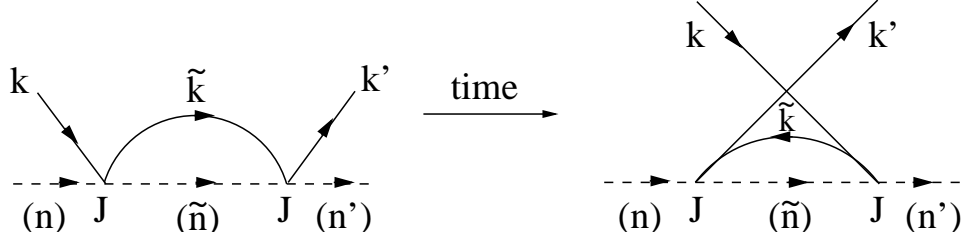


Fig. 1. The basic two logarithmic time ordered diagrams are shown where the solid lines stand for the electrons and the dashed ones for the impurity spins. (In the parenthesis  $n, n', \tilde{n}$  label the excited states in the tunneling problem.)

where  $\alpha$ , in general, is of order of unity due to band structure effects, or by using different upper and lower cutoffs as  $D_{up}$  and  $D_{low}$  instead of  $D$ . Another way<sup>2</sup> to break the e-h.s. is to introduce a local potential  $V\delta(\mathbf{r})$  for the electron e.g. at the impurity site  $\mathbf{r} = 0$ .

The generally accepted approximation has been suggested by Haldane<sup>3</sup> for the case with different  $D_{up} \neq D_{low}$  as

$$\log \frac{D_{up}}{|\omega|} + \log \frac{D_{low}}{|\omega|} = 2 \log \frac{(D_{low}D_{up})^{1/2}}{|\omega|} \quad (5)$$

which only slightly affects the different quantities due to the modified cutoff  $D \rightarrow (D_{low}D_{up})^{1/2}$ .

### 3. KONDO PROBLEM WITH ASYMMETRIC CUTOFF ( $D_{up} \neq D_{low}$ )

The magnetic Kondo problem is described by the Hamiltonian  $H = H_0 + H_I$ , where

$$H_0 = \sum_{\mathbf{k}, \sigma} \varepsilon(\mathbf{k}) a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} \quad (6)$$

and  $a_{\mathbf{k}\sigma}^\dagger$  is the creation operator for an electron with momentum  $\mathbf{k}$ , spin  $\sigma$  and energy  $\varepsilon(\mathbf{k})$ . Furthermore

$$H_I = \sum_{\substack{i=x,y,z \\ \alpha\beta}} J^i \Psi_\alpha^\dagger(0) \sigma_{\alpha\beta}^i \Psi_\beta(0) S^i + V \sum_\alpha \Psi_\alpha^\dagger(0) \Psi_\alpha(0), \quad (7)$$

where  $\Psi_\alpha(0)$  is the electron field operator at the impurity site  $\mathbf{r} = 0$  with spin  $\sigma$ ,  $J^i$  is an anisotropic exchange coupling,  $S^i$  is the spin operator of

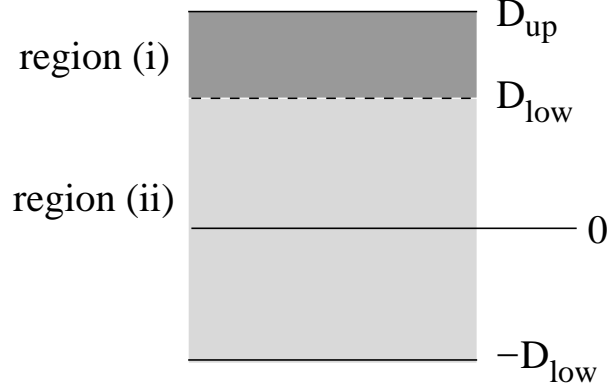


Fig. 2. The energy regions (i) and (ii) due to the asymmetric bandwidth  $D_{up} \neq D_{low}$ .

the impurity, and  $V$  is a static potential at the impurity site. For the most of the cases  $J^i = J$  and  $V = 0$  is taken as the initial values. The two basic logarithmic diagrams are shown in Fig. 1. These contribute as  $\log \frac{D_{up}}{|\omega|}$  and  $\log \frac{D_{low}}{|\omega|}$  with different spin factors  $\pm[S(S+1) \mp \boldsymbol{\sigma} \mathbf{S}]$  where  $\mathbf{S}$  is the spin vector operator of the impurity and  $\boldsymbol{\sigma}$  stands for the vector of Pauli spin matrices of the conduction electrons. In case of  $D_{up} = D_{low}$  the spin diagonal terms corresponding to the diagrams of Fig. 1 are canceling out. That is not the case when we apply a poor man's scaling in two steps for the case  $D_{up} > D_{low}$ <sup>4</sup> eliminating first the energy region (i)  $D_{up} > \varepsilon > D_{low}$  and then (ii)  $D_{low} > \varepsilon > -D_{low}$  (see Fig. 2). In the region (i) only the first diagram in Fig. 1 must be considered, that is actually a one-electron problem and a spin independent part is generated. The scaling equations for the couplings  $J^i$  and  $V$  have the form<sup>4</sup>

$$\frac{d}{dD} \begin{pmatrix} J^x \\ J^y \\ J^z \\ 2V \end{pmatrix} = -\rho_0 \frac{1}{2D} \begin{pmatrix} 2V & -J^z & -J^y & J^x \\ -J^z & 2V & -J^x & J^y \\ -J^y & -J^x & 2V & J^z \\ J^x & J^y & J^z & 2V \end{pmatrix} \begin{pmatrix} J^x \\ J^y \\ J^z \\ 2V \end{pmatrix} \quad (8)$$

The solutions of that equation for  $J^x = J^y = J^z = J$  and for the initial value  $V = 0$  are at the bottom of the region (i) ( $D = D_{low}$ )

$$J_{D=D_{low}} = \frac{J}{4} \left( \frac{3}{1 - \frac{3}{2} J \rho_0 \log \frac{D_{up}}{D_{low}}} + \frac{1}{1 + \frac{1}{2} J \rho_0 \log \frac{D_{up}}{D_{low}}} \right). \quad (9)$$

There is also a potential  $V$  generated, but the latter one does not have a role in the symmetric region (ii).  $J_{D=D_{low}}$  is the initial coupling for the scaling in the region (ii) with cutoff  $D_{low}$ . In the extreme limit  $D_{up} \gg D_{low}$  the

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scaling in region (ii) does not lead to any essential renormalization and the coupling diverges at the Kondo temperature  $T_K$ , which is now

$$T_K = D_{up} e^{-\frac{1}{\frac{3}{2}J\rho_0}}. \quad (10)$$

Thus, having  $D_{low} \ll D_{up}$  results in the change of the exponent  $(2J\rho_0)^{-1}$  to  $(3/2J\rho_0)^{-1}$  and surprisingly  $D_{low}$  drops out. That result is different from the expectation, that half of the diagrams gives coupling with half strength, and, thus, the exponent should be  $(J\rho_0)^{-1}$ . In this result the generated potential scattering inside region (i) plays a crucial role.

Such a limit may be interesting in the cases of degenerate semiconductors with magnetic impurities or tunneling centers<sup>5</sup>.

## 4. THE COMMUTATIVE TUNNELING MODEL E-H.S. BREAKING

A two-level system (TLS) described by a  $\sigma_{TLS}$  Pauli operator is coupled to the spherical electron waves with different angular momenta  $l$ , but only to the azimuthal channel  $m = 0$  in case where the axis of the TLS is chosen to be the  $z$  axis<sup>6</sup>. Keeping only two angular momenta, the structure of the coupling can be decomposed also into Pauli matrices. The simplest such Hamiltonian is

$$H_1 = \sum_{\substack{i=x,y,z \\ \alpha,\beta \\ k,k',\sigma}} V^i \sigma_{TLS}^i a_{k\alpha\sigma}^\dagger (\sigma_{el}^i)_{\alpha\beta} a_{k'\beta\sigma} + \Delta_0 \sigma_{TLS}^x \quad (11)$$

and the real spin  $\sigma$  is a silent (conserved) variable.  $V^z$  describes the screening coupling between the tunneling atom and the electrons,  $V^x$  and  $V^y$  are due to electron assisted transitions considering the TLS. The spontaneous tunneling rate is  $\Delta_0$ . In the so-called commutative model  $V^x = V^y = 0$  and  $V^z$  are not renormalized, the renormalization affects only  $\Delta_0$ .

A. Moustakas and D. Fisher<sup>2</sup> pointed out, that in such a model the potential scattering at the impurity site (see the second term on the right hand side of Eq. (7)) may induce  $V^x \neq 0$ ,  $V^y \neq 0$  due to  $V^z \neq 0$  and  $\Delta_0 \neq 0$  at the initial condition. That problem has been investigated in further details<sup>1</sup>. In the original work<sup>2</sup> bosonization is used which clearly shows general tendencies, but it is hard to connect it to the bare coupling constants, therefore, a systematic diagrammatic study has been performed<sup>1</sup>.

The effect of the local potential scattering  $V$  can be exactly taken into account by solving the one-electron problem in the presence of the potential, and then the e-h.s. breaking generates  $\alpha \neq 0$  in Eq. (4). The  $V^x$  coupling

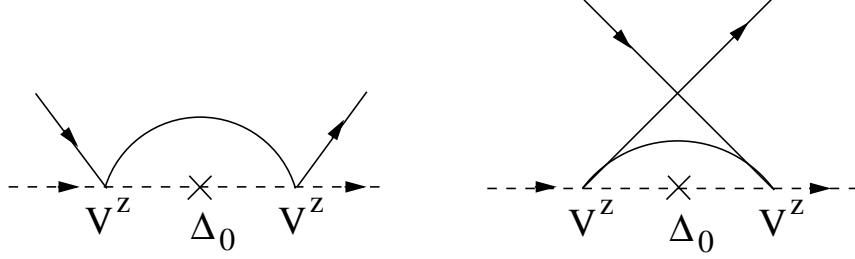


Fig. 3. The diagrams generating the electron-TLS interaction which is off-diagonal in the TLS variables.

can be generated by the typical diagrams shown in Fig. 3. It is easy to show, that the two diagrams in Fig. 3 cancel out if e-h.s exists, thus  $\rho(\varepsilon) = \rho_0$ . Using, however,  $\rho(\varepsilon)$  given by Eq. (4),  $V^x$  is generated by the initial strength  $\frac{\alpha}{D}(V^z)^2\Delta_0$ . One may expect that this non-commutative term can drive the system away from the marginal line  $V^z = \text{const}$ ,  $V^x = V^y = 0$  to the strong coupling isotropic two-channel Kondo fixed point, where  $V^x = V^y = V^z \sim 1$ . But that is not the case, as  $\Delta_0$  plays also the role of an infrared cutoff. Thus,  $\Delta_0$  drives the couplings away from the marginal line and also stops it in its original vicinity (see Fig. 4). Thus, the  $V^x = V^y = 0$  model does not scale to the interesting region with two-channel Kondo behavior with non-Fermi liquid physics. In order to reach that, at least  $V^x \neq 0$  with a significant coupling strength is required. Similar diagrams play a role in the next section.

## 5. ORBITAL TWO-CHANNEL KONDO PROBLEM WITH CHANNEL SYMMETRY BREAKING BY SPIN-ORBIT INTERACTION

TLS's interacting with conduction electrons may represent the two-channel Kondo problem<sup>6</sup> where the channel degeneracy is due to the real spin of the electrons. Motivated by the discrepancies of the results of the two-channel Kondo problem and some experimental data<sup>7</sup>, here we examine the possibility of breaking this degeneracy by the spin-orbit interaction<sup>8</sup>.

We consider a TLS interacting with conduction electrons which are also interacting with a spin-orbit scatterer at a position  $\mathbf{R}$  separated from the TLS (see Fig. 5). The corrections to the conduction electron Green's function due to the interaction with the spin-orbit scatterer in appropriate coordinate systems for the TLS/electron orbital momentum and for the electron spin spaces (see Fig. 5) can be summed up to infinite order, resulting in the

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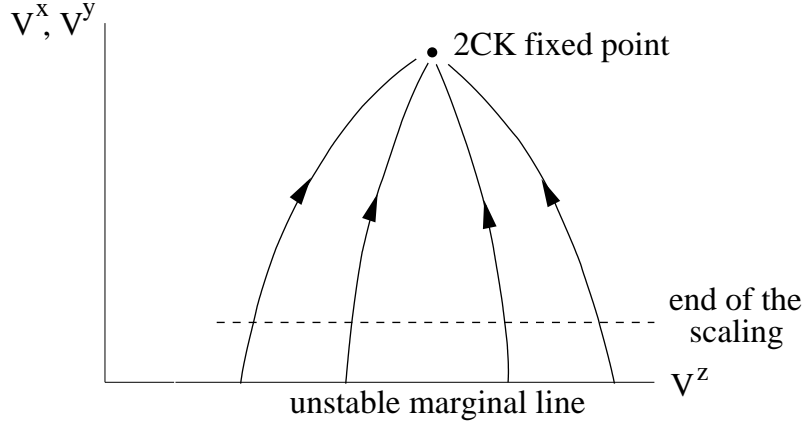


Fig. 4. The scaling trajectories are shown. The marginal line  $V^x = V^y = 0$  is unstable due to the e-h.s. breaking and the trajectories are heading in the direction of the two-channel Kondo (2CK) fixed point. The low energy  $\Delta_0$  restricts the scaling to the region below the dashed line.

following change in the density of states of the conduction electrons<sup>8,9</sup>

$$\frac{\delta\rho_{\mathbf{R}}(\omega)}{\rho_0} = \Lambda\sigma_{l'l}^z\sigma_{\sigma'\sigma}^z, \quad (12)$$

where the correct dispersion given by Eq. (3) was used, i.e. in the density of states  $\alpha \neq 0$  (see Eq. (4)).  $\Lambda$  depends on the strength of the spin-orbit interaction, the energy and the corresponding hybridization matrix element of the orbital where the spin-orbit interaction takes place, and the position  $\mathbf{R}$  of the spin-orbit scatterer according to the TLS. The  $l, l'$  and  $\sigma, \sigma'$  indices correspond to the orbital momentum and the real spin of the conduction electrons, respectively. That treatment shows strong resemblance to the theory where the spin-orbit scattering generates a surface anisotropy for a magnetic impurity nearby the surface<sup>9</sup>.

Redefining the dimensionless TLS-conduction electron couplings ( $v^i = \rho_0 V^i$ ) by multiplying the bare couplings by the spin-dependent density of states (see Eq. (12)), apart from the change  $v^x, v^y, v^z \rightarrow \tilde{v}^x, \tilde{v}^y, \tilde{v}^z = v^z$ , a new kind of coupling is generated<sup>8</sup> in a form

$$\Lambda v^z \sigma_{\sigma'\sigma}^z \sigma_{\alpha'\alpha}^z \delta_{l'l}$$

where the  $\alpha, \alpha'$  indices label the TLS states.

Now we perform a scaling in the leading logarithmic approximation for the general couplings  $v_{\nu\rho}^\mu \sigma_{\alpha'\alpha}^\mu \sigma_{l'l}^\nu \sigma_{\sigma'\sigma}^\rho$  where  $\mu, \nu, \rho = 0, x, y, z$  according to the coordinate systems in Fig. 5. To examine also the role of the e-h.s. breaking

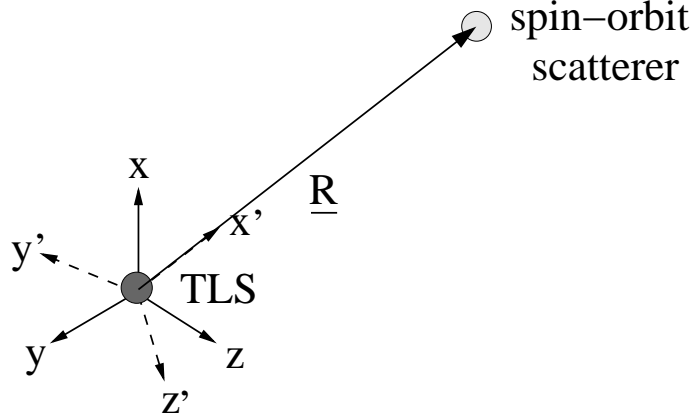


Fig. 5. The TLS and the spin-orbit scatterer. The special  $x, y, z$  (for the TLS and electron orbital momentum spaces) and  $x', y', z'$  (for the electron spin space) coordinate systems with origin at the TLS are also indicated.

in the problem we used Eq. (4) for the conduction electron density of states in the calculation. The leading logarithmic scaling equations are generated by the diagrams in Fig. 1 and 3 with the general couplings at the vertices and the splitting  $\Delta$  and the spontaneous tunneling  $\Delta_0$ <sup>6</sup> at the “crosses” on the TLS line. As the scaling equations with the initial conditions are closed for the subspace  $\rho = 0, z$ , we can restrict the general equations to those values and then define the “average” and the “difference” parts of the couplings as

$$\begin{aligned} v_\nu^\mu &:= \frac{v_{\nu\uparrow}^\mu + v_{\nu\downarrow}^\mu}{2} = v_{\nu 0}^\mu & (\text{average}), \\ \delta v_\nu^\mu &:= \frac{v_{\nu\uparrow}^\mu - v_{\nu\downarrow}^\mu}{2} = v_{\nu z}^\mu & (\text{difference}) \end{aligned} \quad (13)$$

where  $v_{\nu\uparrow}^\mu$  and  $v_{\nu\downarrow}^\mu$  are the couplings for up and down electron spins, respectively. The initial values at  $D = D_0$  are  $v_p^s(0) = \delta_{sp}v_s$ ,  $v_0^s(0) = 0$ ,  $v_p^0(0) = 0$ ,  $\delta v_0^z = \Lambda v^z$ , and the other differences are zero ( $s, p = x, y, z$ ).

After linearization in the differences, the scaling equations for the averages decouple from the others, and it turns out that in leading order in  $\frac{\alpha\Delta}{D}$ ,  $\frac{\alpha\Delta_0}{D}$  the solution for the averages is the usual one<sup>6</sup>, except that couplings  $v_0^s \sim \frac{\alpha\Delta}{D}, \frac{\alpha\Delta_0}{D}$  are generated<sup>8</sup>. Solving the scaling equations for the differences also in first order in  $\frac{\alpha\Delta}{D}, \frac{\alpha\Delta_0}{D}$ , most of the differences remain zero, except  $\delta v_0^z, \delta v_z^x, \delta v_z^y, \delta v_x^z, \delta v_y^z$  where the  $x, y, z$  indices are according to our special coordinate system<sup>8</sup> (see Fig. 5). From the solution of the equations for those couplings we could conclude<sup>8</sup>, that while  $\delta v_0^z$  remains unrenormalized during scaling, the couplings  $\delta v_z^x, \delta v_z^y, \delta v_x^z, \delta v_y^z$  are growing like the usual



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solution for the averages multiplied by  $\frac{\alpha\Delta}{D}$ ,  $\frac{\alpha\Delta_0}{D}$ , but only if  $\alpha \neq 0$ , thus the e-h.s. is broken.

Thus, due to the interaction of the conduction electrons with a spin-orbit scatterer in a position  $\mathbf{R}$  according to the TLS, new, relevant, real spin dependent (thus channel degeneracy breaking) couplings between TLS and conduction electrons are generated in the case of e-h.s. breaking.

The situation is similar to the case presented in Sec. 4.. The e-h.s. breaking breaks the channel symmetry. The crossover between the 2CK and 1CK behavior, however, cannot be reached as the  $\delta v$  terms contain the factor  $\frac{\alpha\Delta}{D}$  or  $\frac{\alpha\Delta_0}{D}$  which is very small. Thus, again the channel symmetry breaking is driven by  $\Delta$  or  $\Delta_0$ , but the same quantities stop the scaling long before the crossover is reached. Thus, this cannot be relevant in the interpretation of the experimental data<sup>7</sup>.

## 6. ELECTRON ASSISTED TRANSITION OF A HEAVY PARTICLE BETWEEN TWO STATES

Considering the interaction between a TLS and electrons the strength of the electron assisted transition is not strong enough to obtain a Kondo temperature  $T_K$  which is required to fit experimental data. It was suggested<sup>10</sup> that the electron assisted transition to excited states with energies above the two lowest levels may give an essential contribution to the electron assisted transition amplitudes  $V^x$  and  $V^y$ , but keeping only a few excited state levels gives unphysical results<sup>11</sup>. Here it is only shown in which sense the argument<sup>11</sup> can be sensitive to e-h.s.<sup>12</sup>. The energy levels of the motion of the localized atom are denoted by  $E_n$ , their wave functions are  $\Phi_n$  and the interaction between the electrons and the atoms is described by the Hamiltonian

$$H' = U \int \Phi_{n'}^\dagger(x) \Phi_n(x) \Psi^\dagger(x) \Psi(x) b_{n'}^\dagger b_n dx, \quad (14)$$

where the local interaction strength is  $U$  and the atom in orbital  $n$  of the potential well is created by the operator  $b_n^\dagger$ . Now again the two diagrams in Fig. 1 should be considered. Consider, e.g., the first diagram. In order to study the scaling equations, the derivative  $D \frac{\partial}{\partial D}$  must be taken, and only the intermediate states with energies  $E_{\tilde{n}} < D$  are contributing. Then the contribution arising from the region of the cutoff  $D$  is (assuming that the wave function of the atom depends on  $z$ ),

$$\sum_{\tilde{n}} \int dz \int dz' e^{i(k_z - \tilde{k}_z)z} \Phi_{\tilde{n}}^*(z) \Phi_n(z) \times \\ e^{i(\tilde{k}_z - k'_z)z'} \Phi_{n'}^*(z') \Phi_{\tilde{n}}(z') \rho(D) \Theta(D - E_{\tilde{n}}), \quad (15)$$

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where  $\omega$  is the incoming energy and  $T = 0$ . As it has been pointed out by Aleiner *et al.*<sup>11</sup>, if  $D$  is large enough, then  $\tilde{n}$  covers a large enough number of states that the approximate sum rule due to approximate completeness of the states,

$$\sum_{\substack{\tilde{n} \\ (E_{\tilde{n}} < D)}} \Phi_{\tilde{n}}(z) \Phi_{\tilde{n}}(z') \sim \delta(z - z') , \quad (16)$$

is satisfied and then the contribution is simplified to

$$\rho(D) \int dz e^{i(k_z - k'_z)z} \Phi_{n'}^*(z) \Phi_n(z). \quad (17)$$

The second diagram has exactly the same contribution but  $\rho(D)$  is replaced by  $-\rho(-D)$ . Thus if  $\rho(D) = \rho(-D)$  holds, there is an exact cancellation. However, that cancellation in the renormalization group equation completely relies on the holding of e-h.s. That is again an example, where results can be essentially affected by breaking the e-h.s.

It is clear, however, that the e-h.s breaking terms do not lead to infrared divergences and can be relevant only in the vicinity of the unrenormalized cutoff. Moving further from the cutoff region the e-h.s. is gradually restored. Thus, the cancellation takes place. The sum of the two diagrams contribute again in the region where the sum rule given by Eq. (16) does not hold, having only a few levels labeled by  $\tilde{n}$ . Thus the e-h.s. breaking has an effect only through the possible enhancement of the couplings entering in the treatment of that second region. That enhancement may be essential for the value of the Kondo temperature.

## ACKNOWLEDGMENTS

Among many of our colleagues we would like to thank especially I. Affleck and B.L. Altshuler for discussing Sec. 3. and Sec. 6., respectively. This work was supported by the OTKA Postdoctoral Fellowship D32819 (O.Ú.) and by Hungarian grants OTKA F030041 (G.Z.), T029813, T030240, and T29236.

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